Towards nanoimprint lithography on free-form surfaces: A global/local modelling approach for predicting the deformation of the flexible stamp

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Towards nanoimprint lithography on free-form surfaces: A global/local modelling approach for predicting the deformation of the flexible stamp

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The work presented in this abstract is a part of the larger EU project called Plast4Future. The aim of this project is to produce injection molding tool inserts with nano-structured functional surfaces. Especially the ability to mimic the colorful nanostructures of the P. blumei butterfly [1] has attracted attention in the plastic industry. But, as the injection moulding tool inserts are non-planar 3-D structures, a flexible stamp is used for the NIL process. As the flexible stamp is stretched and bended during imprint into the curved tool insert, the 3-D deformation of the flexible stamps is essential to take into account, when designing the nano-structures on the 2-D planar silicon wafer. Simulation of this deformation process is performed utilizing a global/local approach. A multi-scale model on two levels is developed: A 3D global model taking care of the overall deformations and stretches of the flexible stamp on the free-form surface, and a coupling to a more local 2D model taking care of the local deformations of the actual nanostructures, see FIG. 2. The coupling between the global and the local model is performed defining the displacements at the edges of a finite element from the global model as boundary conditions in the local model. This is implemented in the general purpose finite elements package ABAQUS. The material used for the flexible stamps is for our purpose polytetrafluoroethylene (PTFE) whose material behavior is described by a constitutive model combining temperature dependent Zenerbody viscoelasticity and Johnson-Cook viscoplasticity [2]. The model is used for simulating nanoimprint of a nanostructure giving a color effect [3] on a double-curved concave steel substrate, see FIG. 1. Both experiment and simulation is found to give a mismatch between the defined and the measured nanostructures (FIG. 3) as a result of the stretch of the flexible stamp during imprint, see FIG. 4. The model is shown to predict the stretch of the nanostructures with a maximum error of 0.5%, indicating that it is able to capture the overall physics of this manufacturing process.

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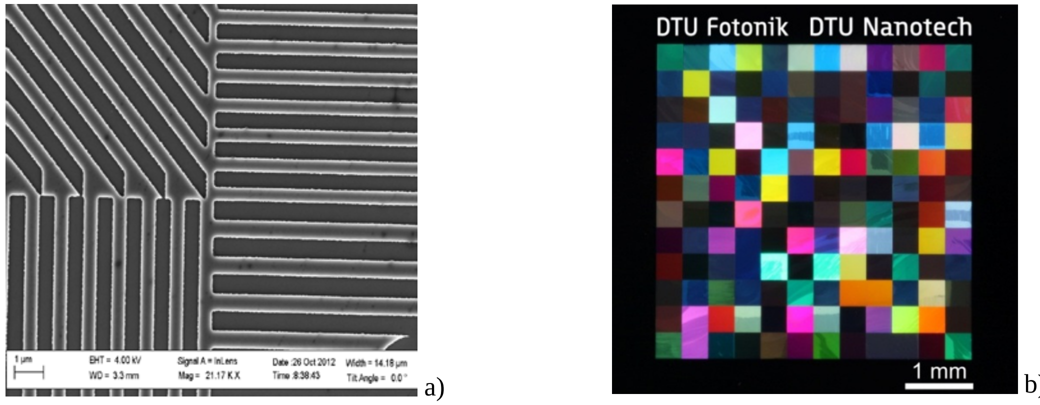

FIG. 1: By combining diffraction gratings with different periods and orientations a glitter-effect can be created. a) Close-up SEM image of the intersection between four different areas with different periods and orientations. b) Photo of glitter sample in black PMMA.

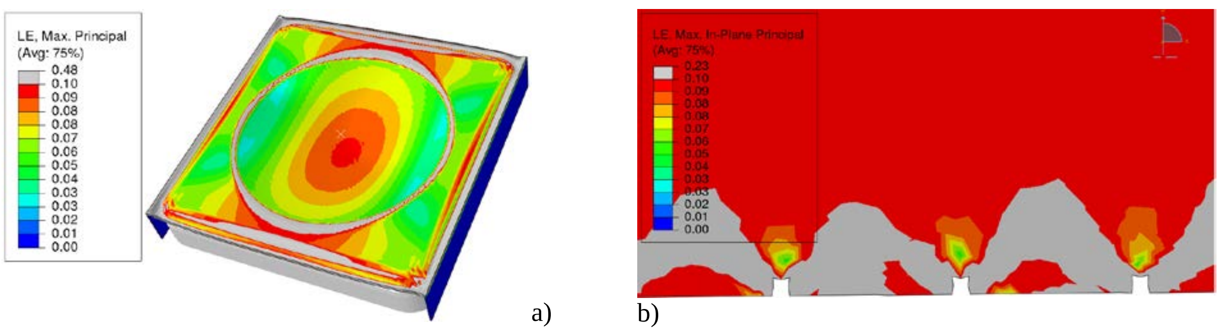

FIG 2: Contourplot of the maximum principal logarithmic strain in a) the global model, b) the nanostructures in the local model, at the final increment of the simulation. The maximum principal strain is the maximum relative stretch in the flexible stamp, which in the middle here is shown to be just above 10%.

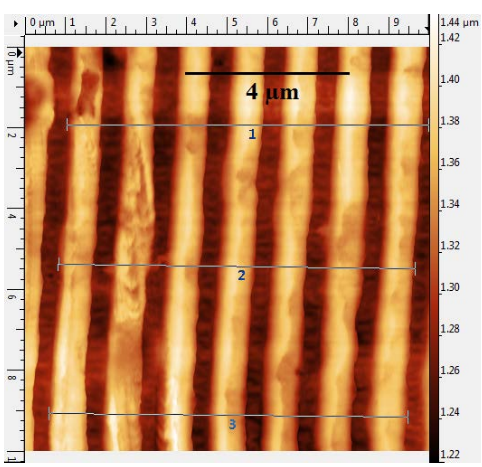

FIG. 3: One of the 32 AFM samples from scanning of a 10x10 µm area. The one dimensional gratings are here seen in 90^{o} orientation. Three profiles are extracted from this scan for comparison with the numerical model.

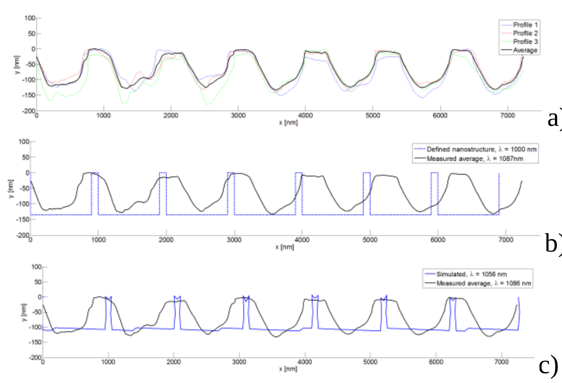

FIG. 4: a) AFM profiles from the 3 profiles shown in FIG. 3. b) Comparison of the measured average profile with the original defined 1000 nm nanostructure. c) Comparison of the measured average profile with the predicted shape of the nanostructures on the deformed flexible stamp.